Quantification of Numerical Uncertainty Via Nonlinear Dynamical Approach

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Motivations

(Ensure a Higher Level of Confidence in the Predictability & Reliability of Numerical Simulation for Multiscale Complex Nonlinear Fluid Problems)

- **The last two decades have been an era when computation is ahead of analysis & when very large scale practical computations are increasingly used in poorly understood multiscale complex nonlinear physical problems & non-traditional fields** ***(Especially when computations offer the ONLY way of generating this type of data limited simulations).***
- **At present some of the numerical uncertainties can be explained and minimized by traditional numerical analysis and standard CFD practices. However, such practices, usually based on linearized analysis, MIGHT NOT be sufficient for strongly nonlinear and/or stiff problems.**
- **We need a good understanding of the nonlinear behavior of numerical schemes being used as an integral part of code verification, validation and certification.**

Major Stumbling Blocks In Genuinely Nonlinear Studies

(Unlike linear model equations used for conventional stability and accuracy considerations in time-dependent PDEs, there are no equivalent unique nonlinear model equations for nonlinear hyperbolic and parabolic PDEs for fluid dynamics)

- On one hand, a numerical method behaving in a certain way for a particular nonlinear PDE might exhibit a different behavior for a different nonlinear PDE even though the PDEs are of the same type.
- On the other hand, even for simple nonlinear model PDEs with known solutions, the discretized counterparts can be extremely complex, depending on the numerical methods.
- Except in special cases, there is no general theory at the present time to characterize the various nonlinear behaviors of the underlying discretized counterparts.

Note:

- ``Discretized counterparts'' is used to mean the finite difference equations resulting from finite discretizations of the underlying PDEs.
- ``Dynamics'' is used loosely to mean the dynamical behavior of nonlinear dynamical systems (continuum or discrete)
- ``Numerics'' is used loosely to mean the numerical methods and procedures for solving dynamical systems.
- In the study of the "Dynamics of Numerics", we usually assume the continuum (governing equations) is nonlinear (*unless the numerical method is nonlinear in solving a linear system*)

Approaches

(Consider the PDE & Its Discretized Counterparts as SEPARATE Dynamical Systems & Analyze them)

- **Based on Knowledge gained for nonlinear model problems with known analytical solutions**
  (Available theory not able to fully analyze nonlinear behavior of numerics for the nonlinear Euler & Navior-Stokes Eqns.)
- **How well numerical methods can mimic the solution behavior of the underlying highly nonlinear PDE model for finite time steps & grid spacings** *(not as they approach zero).*
- **Identify & explain some of the possible sources & remedies of numerical uncertainties in practical computations.**

Spurious Numerics: Solution of Discretized Counterparts but NOT SOLUTION of the PDE

Sources of Nonlinearities

Due to Physics and/or Numerical Methods

Well Known Sources of Nonlinearities are Due to Physics:

Convection, diffusion, forcing, turbulence source terms, reacting flows, combustion related problems, or any combination of the above, etc.

Less Familiar Sources of Nonlinearities are Due to the Numerics -- Three Major Sources:

(1) Nonlinearities due to time discretizations -- discretized counterpart is nonlinear in the time step

> Runge-Kutta methods. If fixed time steps are used, spurious steady-state or spurious asymptotic numerical solutions can occur, depending on the the initial condition (IC).

> Linear multistep methods (LMMs) (Butcher 1987) are linear in the time step, and they do not exhibit spurious steady states. See Yee & Sweby (1991-1997) and references cited therein for the dynamics of numerics of standard time discretizations.

(2) Nonlinearities due to spatial discretizations -- discretized counterpart can be nonlinear in the grid spacing and/or the scheme

E.g., Total variation diminishing (TVD), essentially nonoscillatory (ENO) and weighted ENO (WENO) schemes: The resulting discretized counterparts are nonlinear (in the dependent variables) even though the governing equation is linear.
See Yee et al. (1989) references cited therein for the early forms of these schemes.

(3) Nonlinearities due to complex geometries, boundary interfaces, grid generation, grid refinements and grid adaptations

See, Yee & Sweby 1995 -- *each of these procedures can introduce nonlinearities Even though the governing equation is linear.*

Selected Results on Different Nonlinear Behavior of Numerical Methods

(Spurious dynamics INDEPENDENTLY *introduced by* Spatial & Time *discretizations)*

Spurious Numerics Due to Time Discretizations:

- Occurrence of stable and unstable spurious asymptotes ABOVE the linearized stability limit of the scheme (for constant time steps)
- Stabilization of unstable steady states by implicit and semi-implicit methods
- Interplay of initial data and time steps on the occurrence of spurious asymptote
- Interference with the dynamics of the underlying implicit scheme by procedures in solving the nonlinear algebraic equations *(resulting from implicit discretizations of the continuum equations)*
- Dynamics of the linearized implicit Euler scheme solving the time-dependent equations to obtain steady states vs. Newton's method solving the steady equation
- Etc.

Spurious Numerics Due to Spatial Discretizations:

- Convergence problems & spurious behavior of high-resolution shock-capturing methods
- Numerically induced & suppressed (spurious) chaos & numerically induced chaotic transients
- Spurious dynamics generated by grid adaptations
- False Numerical Prediction of Transition to Turbulence
- Wrong propagation speed of discontinuities for problems containing stiff source terms, etc.

Methods of Lines (MOL) Approach

In General, MOL Approach is Easier to Analyze than Mix Time & Space Approaches:

- **Spurious Numerics due to Time Discretizations are Easier to Overcome by, e.g., Adaptive Time Step Control**
- **Spurious Numerics due to Spatial Discretizations are More Difficult to Overcome even by, e.g., grid refinement, adaptation and/or multigrid approaches**

Knowledge Gained from Spurious Numerics Due to Spatial Discretizations Leading to the Need:

- **Adaptive Numerical Dissipation Controls for Long Time Integration of Unsteady Flows: Direct Numerical Simulations (DNS), Large Eddy Simulations (LES), Simpletic Dynamical Systems, etc.**
- **Physical Preserving (Structural Preserving) Methods**
- **Improvement in nonlinear Stability & Accuracy by High Order Skew Symmetric Splitting of the Inviscid Flux Derivatives**
- **Numerical Treatment of Source Terms and Nonlinear Stiff Source Terms**
- **Etc.**

Spurious Numerics Due to Source Terms

Phenomena occur in simple scalar case – 3D complex systems

Source Terms: Hyperbolic conservation laws with source terms

> Most high order shock-capturing schemes are NOT well-balanced & produce huge error

> High order WENO/Roe & their nonlinear filter counterparts are well-balanced for certain reacting flows **Our Work:** Wang et al. JCP papers 2010, 2011

Stiff Source Terms:

> Numerical dissipation can result in wrong propagation speed of discontinuities for under-resolved grids if the source term is stiff LeVeque & Yee, 1990

> This numerical issue has attracted much attention in the literature – last 27 years (Improvement can easily be obtained for a single reacting flow case)

> A New Sub-Cell Resolution Method has been developed for stiff systems on coarse mesh **Our Work:** Wang et al., JCP, 2012 ; CiCP 2016

Nonlinear Source Terms:

> Occurrence of spurious steady-state & discrete standing-wave solutions – by the use of fixed grid spacings & time steps or grid adaptation Yee & Sweby, Yee et al., Griffiths et al., Lafon & Yee, 1990-2002

Stiff Nonlinear Source Terms with Discontinuities:

> More complex spurious behavior

> Forced Turbulence, numerical combustion, certain terms in turbulence modeling & reacting flows Yee et al., Yee & Sweby, Griffiths et al., Lafon & Yee, Kotov et al. 1990 – 2017

Selected Illustration

- **Spurious Numerics Due to Stiff Nonlinear Source Terms**
- **Physical Preserving High Order Numerical Methods for Turbulence with Shocks**

  E.g., ***Entropy Conserving, Momentum Conserving, Kinetic Energy Preserving, Positivity Preserving, Skew-Symmetric Splitting to Improve Nonlinear Stability without ADDING Numerical Dissipation***

1D C-J Detonation Wave

(Helzel et al. 1999; Tosatto & Vigevano 2008)

Left state (totally burned gas)	**Right state (totally unburned gas)**

$$\begin{pmatrix}\rho_b\\ u_b\\ p_b\end{pmatrix} = \begin{pmatrix}\rho_u \dfrac{[p_b(\gamma+1)-p_u]}{\gamma p_b}\\ S_{CJ}-(\gamma p_b/\rho_b)^{1/2}\\ -b+(b^2-c)^{1/2}\end{pmatrix} \qquad \begin{pmatrix}\rho_u\\ u_u\\ p_u\end{pmatrix} = \begin{pmatrix}1\\ 0\\ 1\end{pmatrix}$$

$$S_{CJ} = [\rho_u u_u + (\gamma p_b \rho_b)^{1/2}]/\rho_u$$

$$b = -p_u - \rho_u q_0(\gamma-1) \qquad c = p_u^2 + 2(\gamma-1)p_u\rho_u q_0/(\gamma+1)$$

Ignition temperature $T_{ign} = 25$

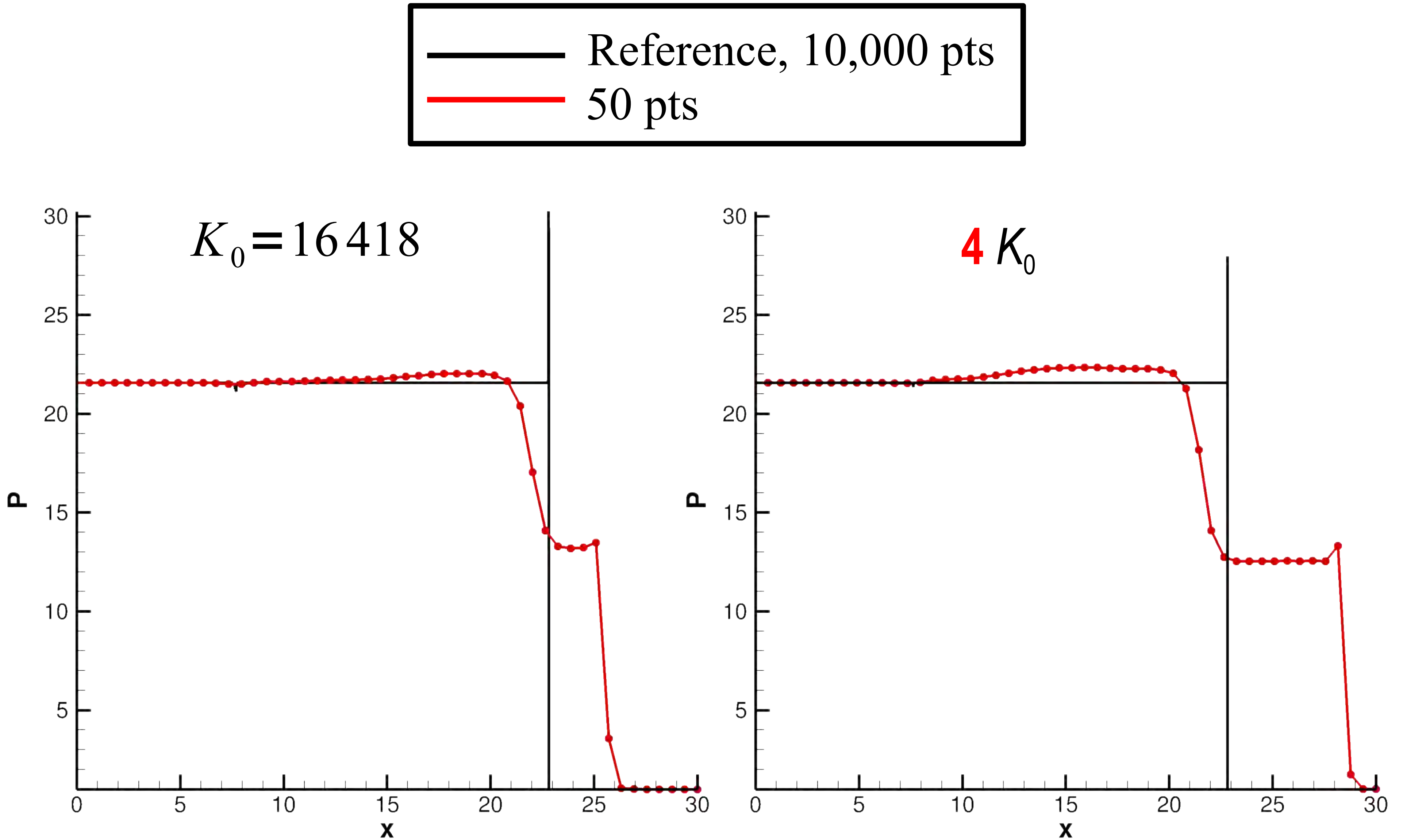
Heat release $q_0 = 25$

Rate parameter $K_0 = 16418$

$$K(T) = K_0 \exp\left(\frac{-T_{ign}}{T}\right)$$

Wrong Propagation Speed of Discontinuities

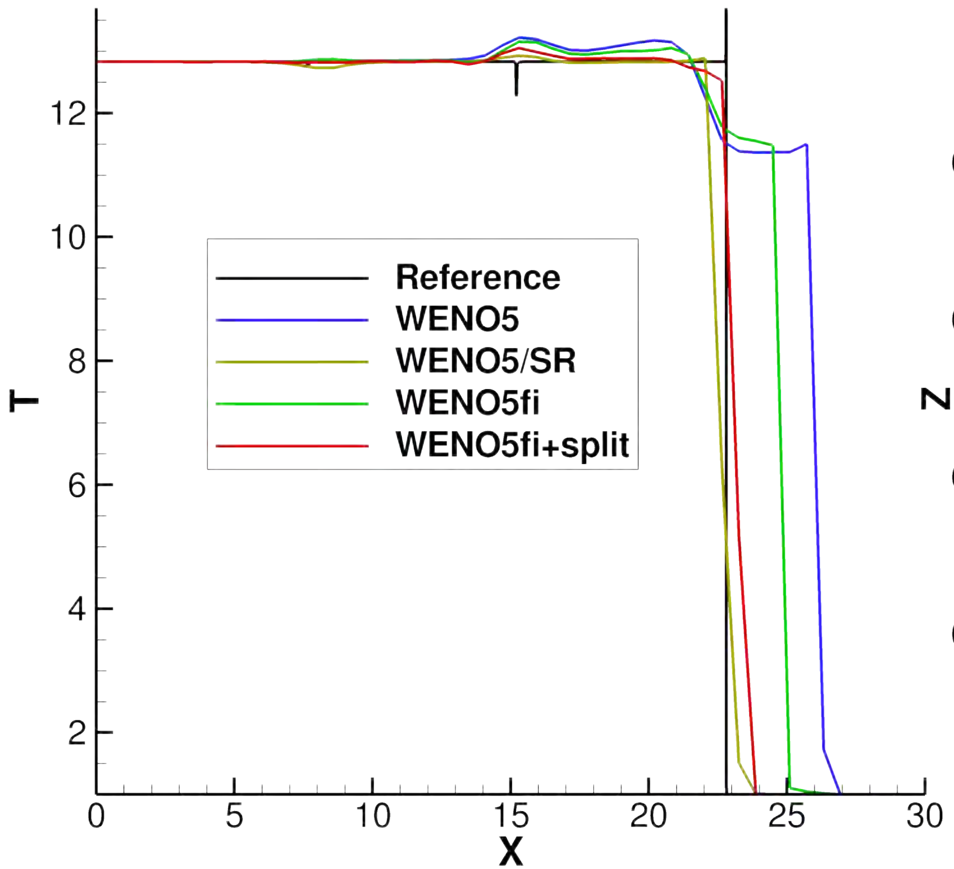
(WENO5, Two Stiff Coefficients, 50 pts)



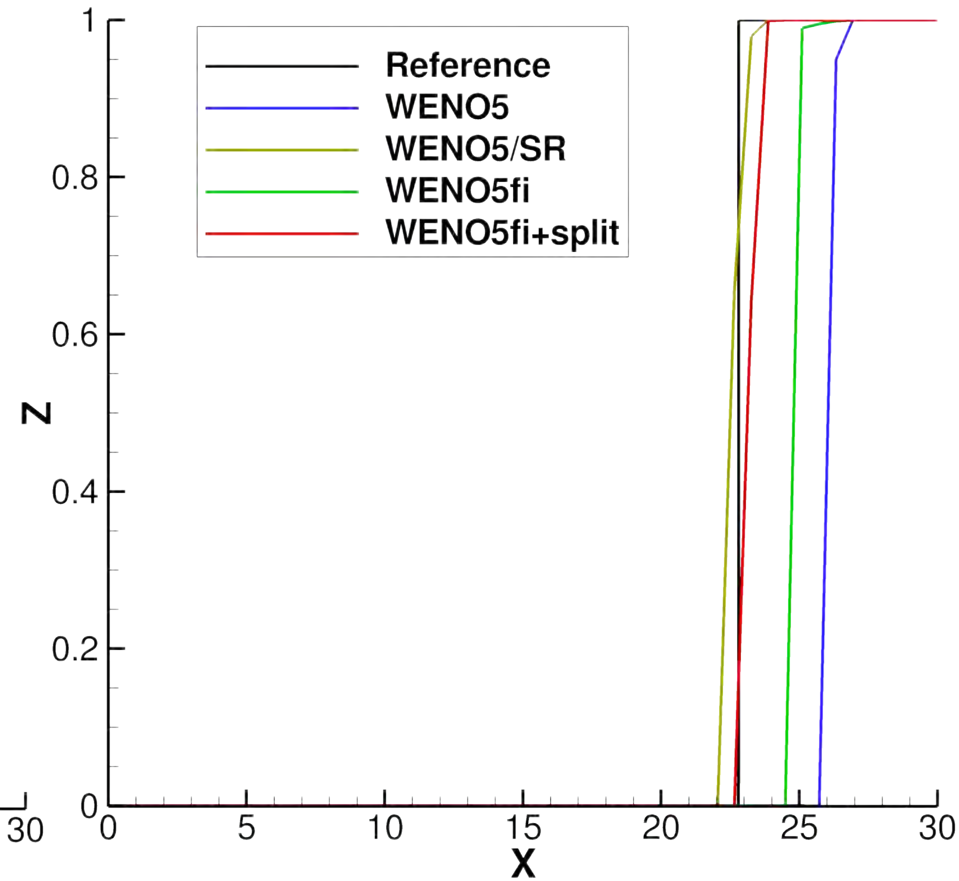
1D C-J Detonation (K_0 = 16418, 50 pts)

tend = 1.7

Temperature



Mass Fraction



Standard Meth. – WENO5: Standard 5^{th} order WENO (WENO7, TVD)

Improved Meth. –
- WENO5/SR: WENO5 + subcell resolution
- WENO5fi: filter version of WENO5
- WENO5fi+split: WENO5fi + preprocessing (Ducros splitting)

Reference: WENO5, 10,000 points

(Strang Splitting & Safeguard)

Scalar Case Behavior of WENO5 & WENO5/SR below CFL limit

Source term:

$S = K_0(1\text{-}u)(u\text{-}0.5)u$

$K_0 = 10{,}000$

(Obtaining the Correct Discontinuity Speed)

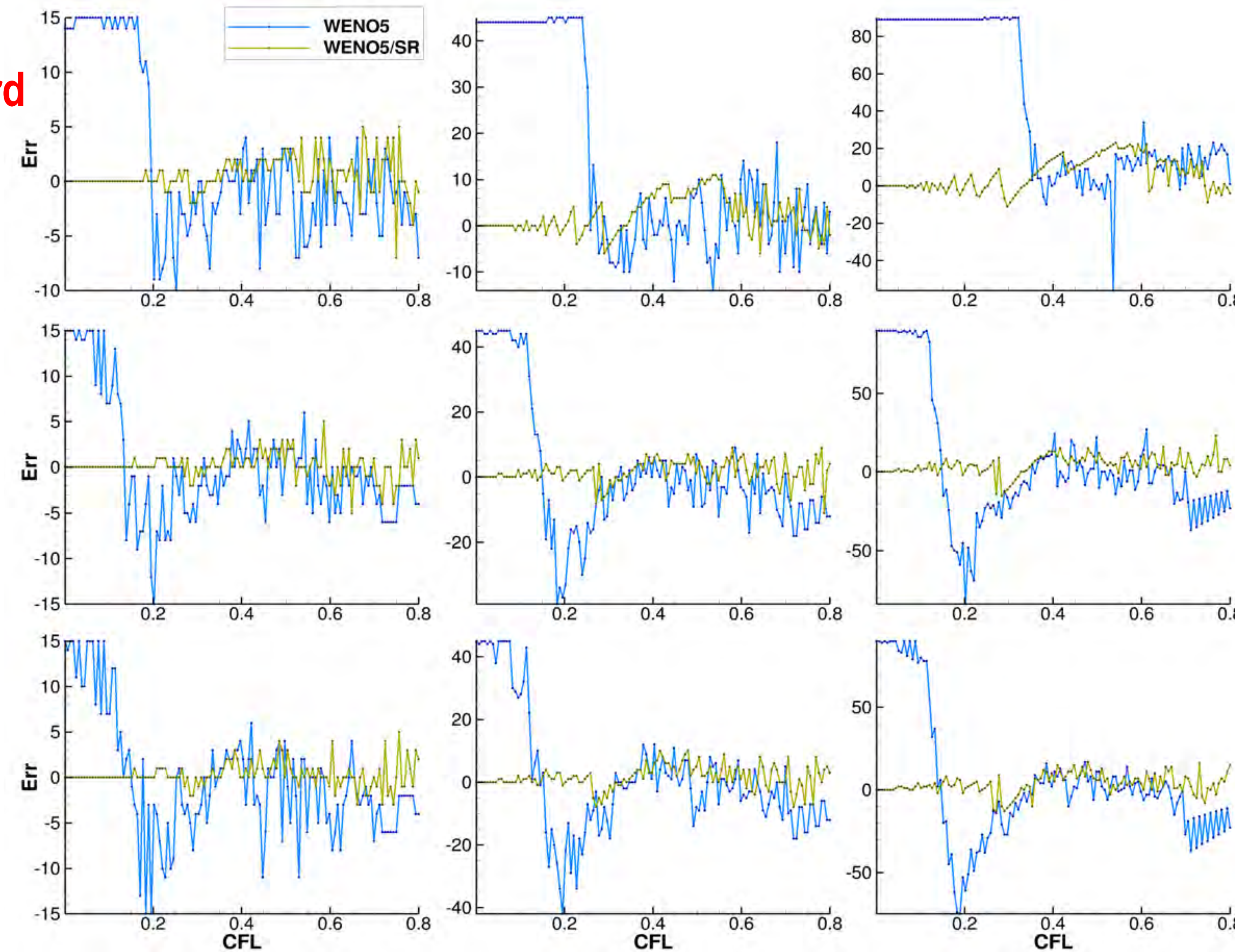
Strang/Safeguard

Grid 50 | Grid 150 | Grid 300

Stiff. K_0

Stiff. 100 K_0

Stiff. 1000 K_0



Note: CFL limit based on the convection part of PDE

Effort of Different Time Integrator -- Reaction Step

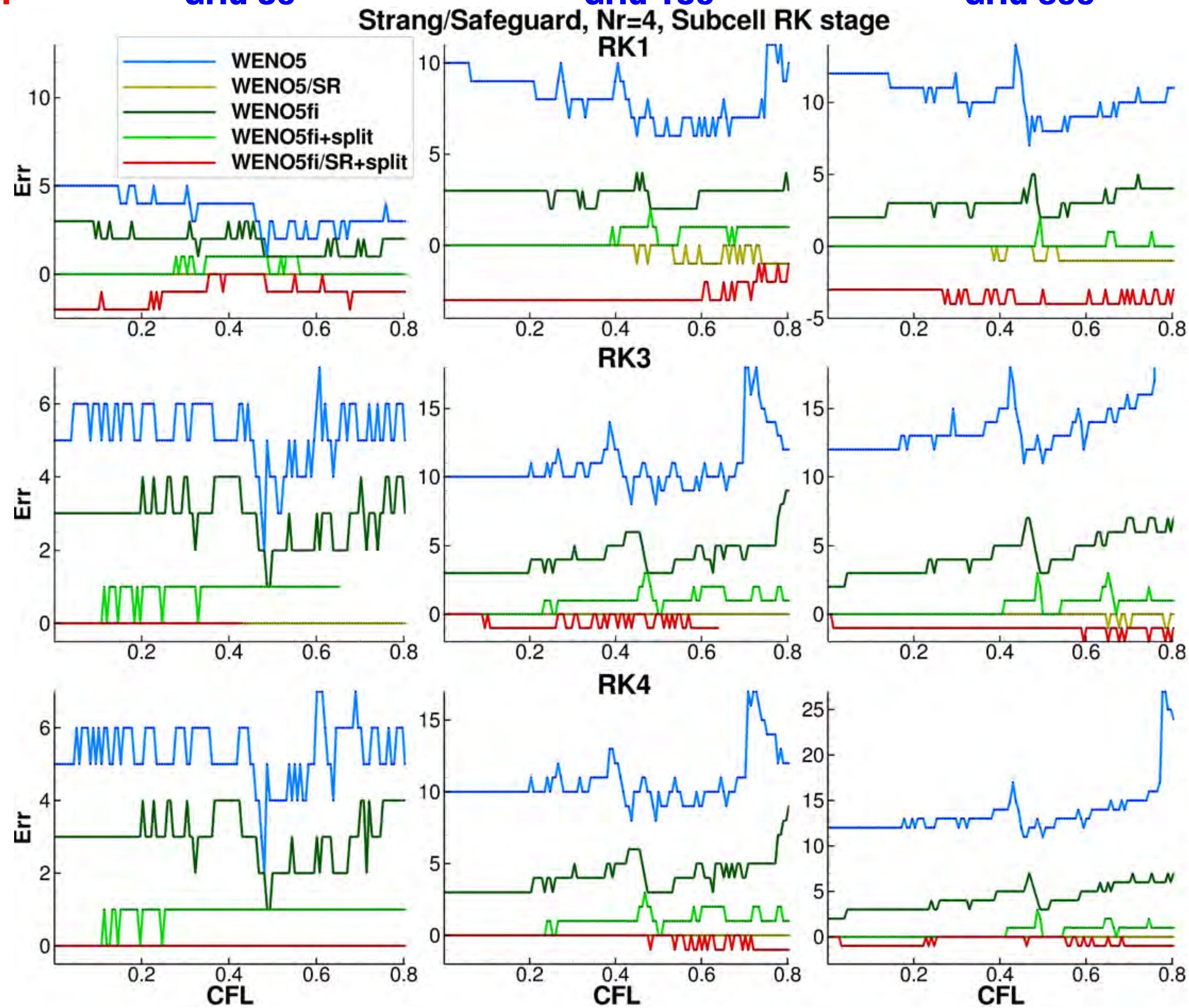
(Strang Splitting/Safeguard, Nr=4, SR at every RK stage)

1D C-J Detonation **Grid 50** **Grid 150** **Grid 300**

RK1

RK3

RK4



Scalar Case Behavior of WENO5 & WENO5/SR below CFL limit

(Obtaining the Correct Discontinuity Speed)

Source term:

$S = K_0(1\text{-}u)(u\text{-}0.5)u$

$K_0 = 10{,}000$

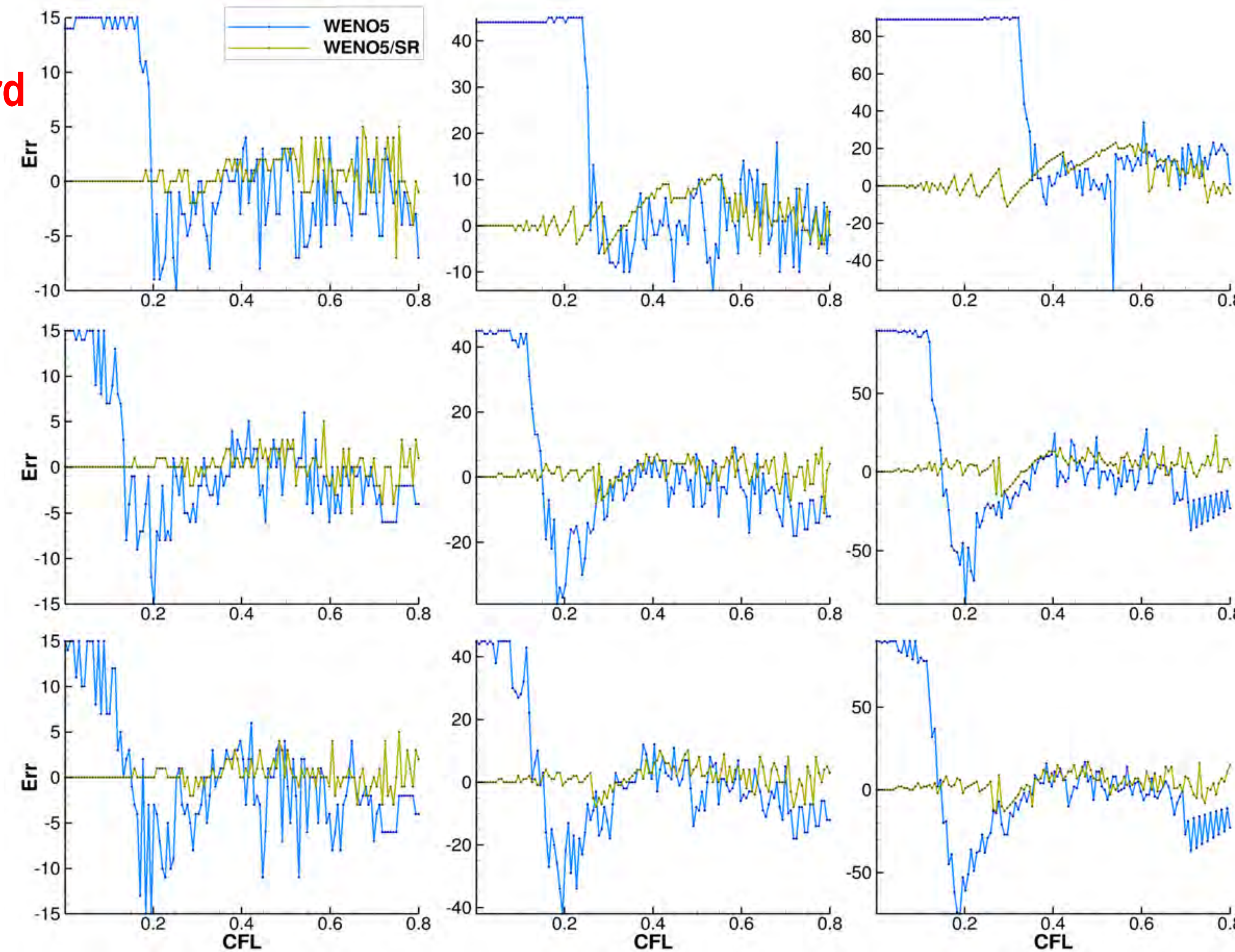
Strang/Safeguard

Grid 50 **Grid 150** **Grid 300**

Stiff. K_0

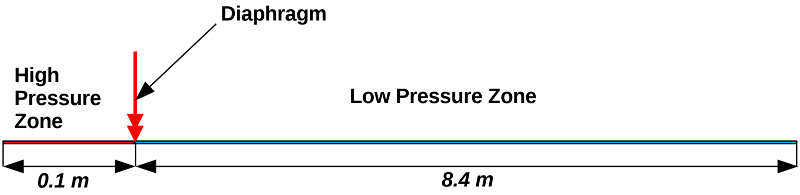
Stiff. 100 K_0

Stiff. 1000 K_0



Note: CFL limit based on the convection part of PDE

1D EAST Problem Setup



13 species mixture:

$$e^-, He, N, O, N_2, NO, O_2, N_2^+, NO^+, N^+, O_2^+, O^+, He^+.$$

High Pressure Zone

ρ	$1.10546\ kg/m^3$
T	$6000\ K$
p	$12.7116\ MPa$
Y_{He}	0.9856
Y_{N_2}	0.0144

Low Pressure Zone

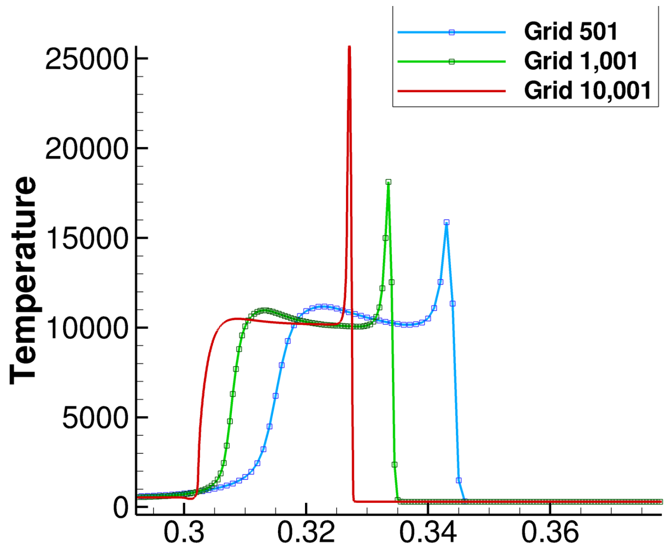
ρ	$3.0964 \times 10^{-4} kg/m^3$
T	$300\ K$
p	$26.771\ Pa$
Y_{O_2}	0.21
Y_{N_2}	0.79

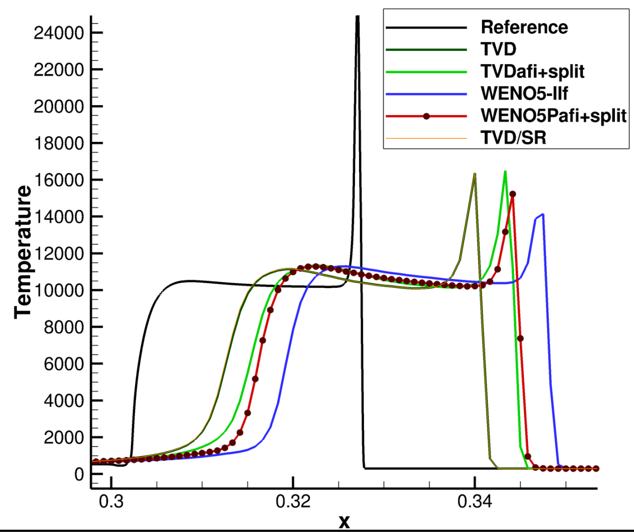
Stiff Source Terms: Wrong Discontinuity Locations

(Grid & method dependence of shock/shear locations)

NASA *Electric Arc Shock Tube* (EAST)

- 1D Computation: 13 species(Air+He) using MUTATION library; L = 8.5 m
- Fine grid step h = 0.05mm, 16 times finer than coarse grid





Flows without stiff source term: Computed locations of discontinuities are independent of the grid size or high-resolution shock-capturing methods

Implication: The danger in trusting numerical simulation for problems with stiff source terms

Non-standard behavior of numerics observed in non-reacting flows

(Yee et al., Griffith et al., Wang et al., Kotov et al., 1990 - 2016)

Challenges in Numerical Method Development

(Long Time Integration of Multiscale Compressible Turbulence)

Nonlinear Instability:

> Existing accurate schemes developed for rapidly developing flows usually SUFFER from nonlinear instability for long time integration

Numerical Stability & Accuracy: Conflicting Requirements for DNS & LES

> Stable schemes usually contain more numerical dissipation than their higher accuracy counterparts

> Numerical dissipation usually smears turbulent fluctuations

> Proper amount of numerical dissipation is required for stability in the vicinity of discontinuities

Difficult to Resolve All Scales: Need efficient methods with extremely fine grids & CPU intensive

Source Terms:

> Well-balanced schemes are needed to preserve physical steady states exactly

> Numerical dissipation & under-resolved grids lead to incorrect shock speeds if source term is stiff

Problems Containing a Wide Spectrum of Flow Speeds & Flow Types:

> Forced compressible turbulence can initially start with shock-free turbulence but might develop moderate to strong shock waves at a later time (Kotov et al. JCP, 2016)

> Cannot be solved accurately with standard numerical methods

Our New Development to address these challenges:
(Yee et al., Yee & Sjogreen, Sjogreen & Yee, Wang et al., Kotov et al., 2009-2018)

Physical Preserving (Structural Preserving) Methods are Essential in Minimizing Spurious Numerics

Methods to Improve Nonlinear Stability & Accuracy

(Long Time Wave Propagation & Long Time Integration of Compressible Turbulence)

- Skew-Symmetric Splitting of the inviscid flux derivative (before the application of non-dissipative centered schemes for nonlinear stability) Yee & Sjogreen, Sjogreen & Yee, 2016-2018

- DRP (Dispersion Preservation-Relation) schemes as alternatives to split version of classical high order central schemes Yee & Sjogreen, 2017

- High-Order Entropy Conservative Numerical Fluxes with entropy satisfying properties
  - Numerical solution satisfies an additional discretized conservation law Sjogreen & Yee, 2016-2018

- Standard high order Linear Filters are to be replaced by high order Nonlinear Filters

  Yee et al., Yee & Sjogreen, Sjogreen & Yee, Kotov et al. (1999-2017)

- Smart Flow Sensors to provide locations & appropriate amount of numerical dissipation needed Yee & Sjogreen, Kotov et al. (2009-2016)

- Nonlinear Dynamics is utilized to complement the traditional linearized stability theory (Yee & Sweby, Yee et al., Griffiths et al., Lafon & Yee, Wang et al., Kotov et al. 1990- 2015)
  - Minimize numerically induced false transition to turbulence
  - Minimize numerical instability due to long time integration of turbulent flows

Yee et al. high-order nonlinear filter schemes with smart local flow sensors

Skew-Symmetric Splitting of Inviscid Flux Derivatives

(Improve nonlinear stability for high order central schemes)

Olsson & Oliger 1994, Yee et al. 1999, Ducros et al. 2000, Pirozzoli 2009, Sjogreen et al. 2017

- **Entropy splitting:** Semi-conservative splitting for shock-free turbulence
  (Olsson & Oliger 1994, Yee et al. 1999-2007, Sandham et al. 2002-present)
- **Natural Splitting:** Linearized Euler & Non-conservative Systems
- **Splitting to Preserve Discrete:** Momentum and/or Energy
  (Arakawa 1966, Blaisdell et al. 1996, Mansour 1980, etc.)
- **Ducros et al. Type Conservative Splitting:** Euler & MHD (Sjogreen et al. 2017)
- **Generalized Skew-Symmetric Splitting:** 3-parameter family (Pirozzoli 2009)

Preprocessing Step: Improve stability of classical central scheme

Replacing high order classical central approximation of the inviscid flux derivative
➔ High order approximation of their split form counterpart

High Order Entropy Conservative Methods

(One way to improve nonlinear stability & minimize added numerical dissipation)

- Numerical solutions satisfy additional discretized conservation law
- Low order entropy conservative methods with linear numerical dissipation for shock-capturing require further accuracy improvement
  (Tadmor 1984 – gas dynamics, Janhunen 2000 – MHD, Winters & Gassner 2016 – MHD)
- High order entropy conservative methods for central schemes
  (Fjordholm et al. 2012 – ENO, Carpenter et al. 2013-2016,
  Sjogreen & Yee 2016, 2017– central + nonlinear filter, gas dynamics & MHD)

Plasma (Hypersonic Flows):

Four forms of the MHD equations to be considered

> Conservative form
> Godunov/Powell symmetrizable form (non-conservative)
> Janhunen form: (Div B) terms not included in the gas dynamics part of the equations
> Brackbill & Barnes form

Three forms of the entropy fluxes to be considered

(Winter & Gassner 2016, Chandrasheka & Klingenbery 2016, Sjogreen & Yee 2016-2017)

Comparison Among Seven 8th-Order Methods

- **ECLOG**: Tadmor-type entropy conserving method using the Tadmor entropy function $E_L = -\rho \log(p\rho^{-\gamma})$.

- **ECLOGKP**: Tadmor-type entropy conserving method using the Tadmor entropy function with Ranocha's kinetic energy preserving modification [32].

- **ECHKP**: Entropy conserving using the Harten class of entropy functions $E_H = -\frac{\gamma+\alpha}{\gamma-1}\rho(p\rho^{-\gamma})^{\frac{1}{\alpha+\gamma}}$ [50, 23]. In its base form also satisfies Ranocha's kinetic energy preservation condition (KEP); only one variant for this method [43, 32].

- **KGP**: Kennedy-Gruber-Pirozzoli (KGP) skew-symmetric splitting of the inviscid flux derivative that is kinetic energy preserving [26, 31, 13].

Comparison Among Seven 8th-Order Methods *(Cont.)*

- **ESSW**: Entropy split with Ducros et al. splitting but switch to regular central near discontinuities [46].

- **DSKP**: Ducros Split with KEP.

- **DS**: Momentum conserving Ducros et al. skew-symmetric split of the inviscid flux derivative [14].

2D Isentropic Vortex Convection

(Inviscid, pure convection of the IC)

Computational Domain: Period BC, $0 \le x \le 18, 0 \le y \le 18$

Initial Condition:

$$\rho(x,y) = ((1 - \frac{(\gamma-1)\beta^2}{8\gamma\pi^2} e^{1-r^2})^{\frac{1}{\gamma-1}}$$

$$u(x,y) = u_\infty - \frac{\beta(y-y_0)}{2\pi} e^{(1-r^2)/2}$$

$$v(x,y) = v_\infty + \frac{\beta(x-x_0)}{2\pi} e^{(1-r^2)/2}$$

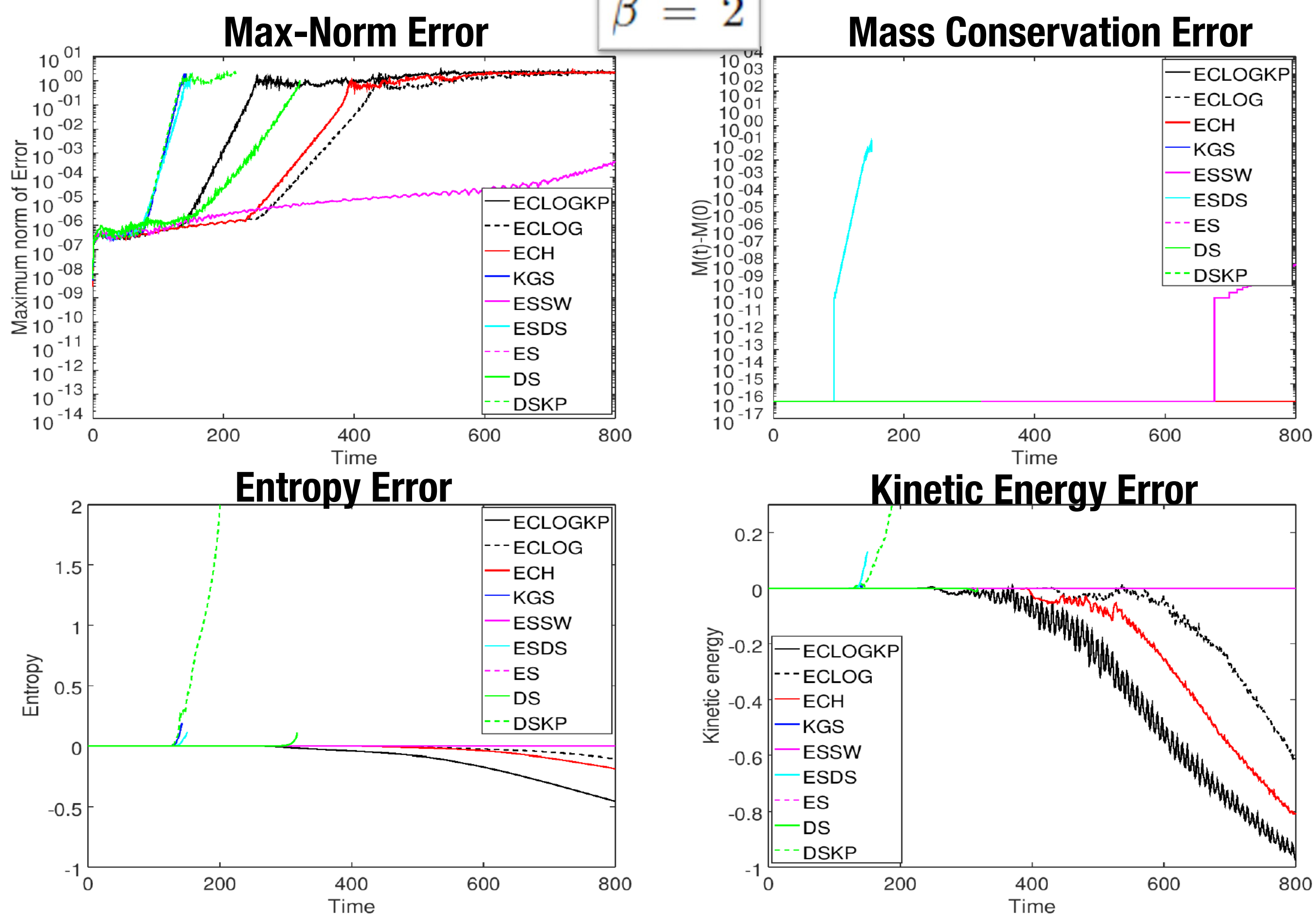
$$p(x,y) = \rho(x,y)^\gamma,$$

$$r^2 = x^2 + y^2, \beta = 5, \gamma = 1.4, u_\infty = 1, v_\infty = 0.$$

2D Isentropic Vortex Convection

Nine 8th-order method comparison, 201^2 grid

$$\beta = 2$$



2D Alfven Wave Test Case

$$\rho = 1 \;\; p = 1 \;\; \mathbf{v} = A(-\sin\alpha\sin\phi,\; \cos\alpha\sin\phi,\; cos\phi)$$

$$\mathbf{B} = (\cos\alpha - A\sin\alpha\sin\phi,\; \sin\alpha + A\cos\alpha\sin\phi,\; Acos\phi)\;\; .$$

$$\phi = 2\pi(x\cos\alpha + y\sin\alpha + t)$$

where $\alpha = 30^\circ$ and $A = 0.1$ are chosen with periodic boundary conditions

==

The computational domain is 1.3546×2.1915

The flow is solved up to time 300 until all methods eventually diverge.

$\Delta x = \Delta y = 0.022$

$\Delta x = \Delta y = 0.011$

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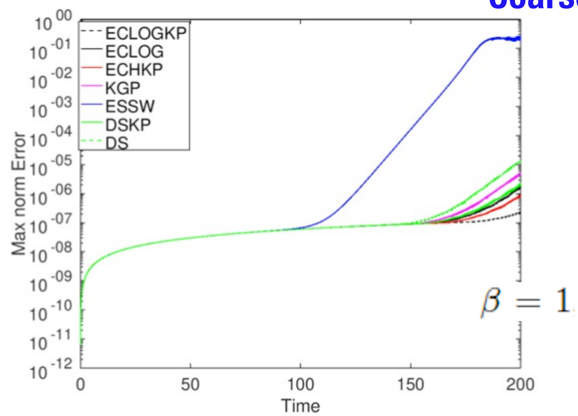
Alfven Wave (Max-Norm Error vs. Time)

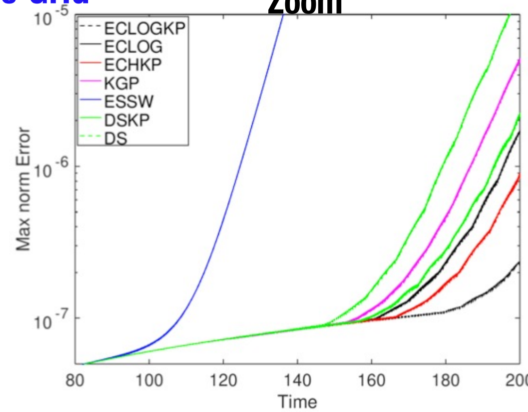
(Comparison Among Seven 8^{th}-order Methods)

$\beta = 1$

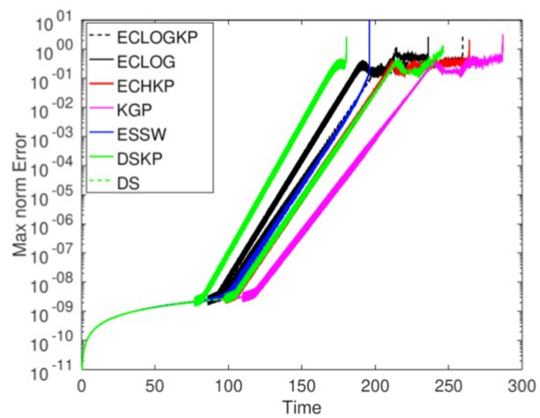
Coarse Grid



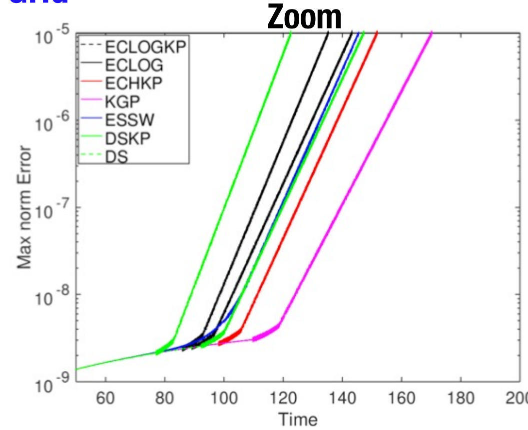
Zoom



Fine Grid



Zoom



Brio-Wu MHD Shock Tube Problem

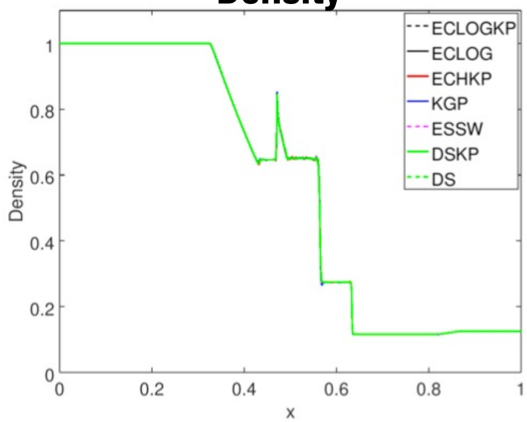
$$(\rho_L,\ u_L,\ p_L,\ B^{(x)},\ B^{(y)},\ B^{(z)}) = (1,\ 0,\ 1,\ 0.75,\ 1,\ 0)$$

$$(\rho_R,\ u_R,\ p_R,\ B^{(x)},\ B^{(y)},\ B^{(z)}) = (0.125,\ 0,\ 0.1,\ 0.75,\ -1,\ 0).$$

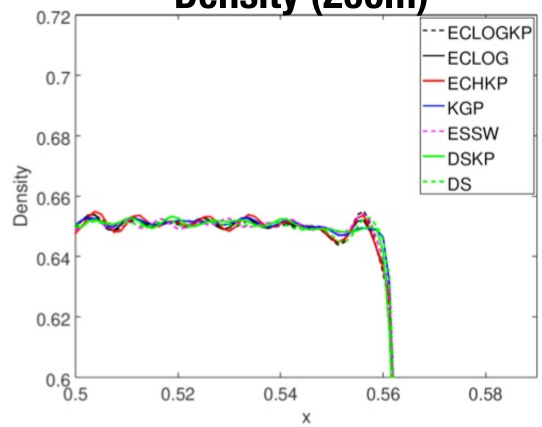
Brio-Wu MHD Shock Tube Problem

(Comparsion Among Seven Methods + 7th-order nonlinear filter)

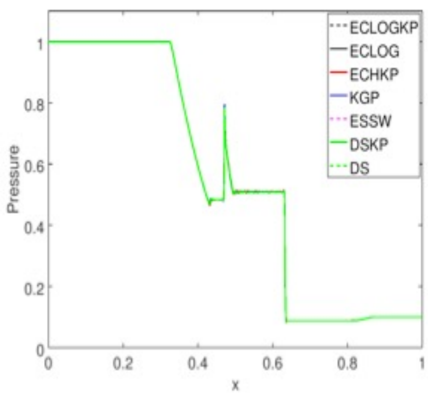
Density



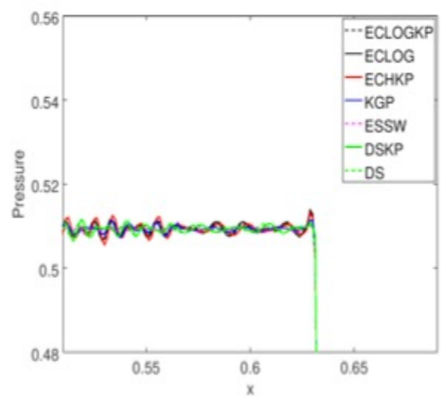
Density (Zoom)

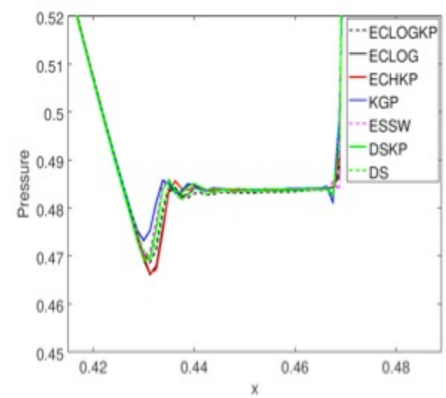


Pressure



Pressure (Zoom)





Brief Summary on Physcial Preserving High Order Methods

GAS dynamics: Classical, DRP and Pade' Spatial discretizations

- All split methods can improve nonlinear stability for smooth flows
  (Without added numerical dissipation in certain flows)
- All nonlinear filter versions of split methods can improve stability & accuracy for DNS & LES
- All split methods provide similar stability & accuracy improvement
  (Pade' methods are most CPU intensive & not friendly in parallelization for multi-D flows)
- All split methods are less CPU intensive than the Tadmor-type entropy conserving methods

Plasma: Classical & Pade' spatial discretizations

- Both split methods can improve nonlinear stability in general for smooth flows but are MHD equations dependent (Pade' methods are most CPU intensive & not friendly in parallelization for multi-D flows)
- Nonlinear filter version of split schemes can improve stability & accuracy for flows with discontinuities but are MHD equations dependent
- High order entropy conserving methods (centered or nonlinear filter version) can provide different stability & accuracy improvement, depending on the forms of the MHD equations & the choice of entropy fluxes

Key Overview References Related to Our Work

- Yee, H.C. and Sweby, P.K. (1997), ``Dynamics of Numerics & Spurious Behaviors in CFD Computations,'' Keynote paper, 7th ISCFD Conference, Sept. 15-19, 1997, Beijing, China}, RIACS Technical Report 97.06, June 1997.
- Yee, H.C. and Sjogreen, B., (2001c) ``Building Blocks for Reliable Complex Nonlinear Numerical Simulations,'' Turbulent Flow Computation, (Eds. D. Drikakis & B. Geurts), Kluwer Academic Publisher; also RIACS Technical Report, Dec. 2001.
- Yee, H.C., Kotov, D.V., Wang, W., and Shu, C.-W. (2013) "Spurious Behavior of Shock-Capturing Methods by the Fractional Step Approach: Problems Containing Stiff Source Terms and Discontinuities," J. Comput. Phys}, 241, 266-291.
- Kotov, D.V., Yee, H.C., Pansei, M., Prabhu, and Wray, A.A. (2014) "Computational Challenges for Simulations Related to the NASA Electric Arc Shock Tube (EAST) Experiments," J. Comput. Phys. 269, 215-233.
- Yee, H. C., Sjogreen, B. (2022): Recent Advancement of Entropy Split Methods for Compressible Gas Dynamics and MHD. J. Appl. Math. Comput., A special issue in the Journal of Applied Mathematics and Computation (ACM) on Hyperbolic PDE in computational physics: Advanced Mathematical Models and Structure-Preserving Numerics.

List of Our Publications Related to This Talk

Request from H.C. Yee: Helen.M.Yee@ nasa.gov